

## LA-UR-21-30688

Approved for public release; distribution is unlimited.

Title: Safety Applications Project FY20-21 Highlights, FY22 Goals

Author(s): Smith, Brandon Michael

Intended for: Project Update

Issued: 2021-10-27

---

**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

UNCLASSIFIED



# Safety Applications Project FY20-21 Highlights, FY22 Goals

Brandon Smith  
October 21, 2021



Managed by Triad National Security, LLC., for the U.S. Department of Energy's NNSA.

UNCLASSIFIED

# Outline

- **Highlights**
- **Collaborations**
- **Capabilities**
- **Infrastructure**
- **Performance**



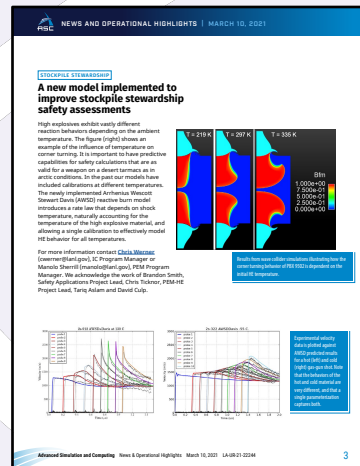
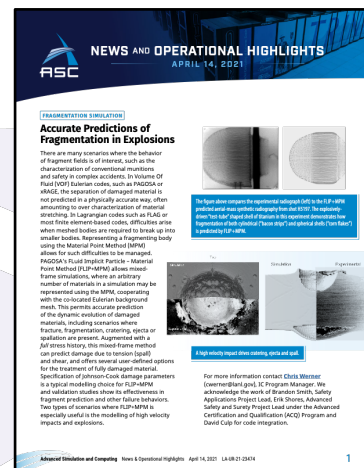
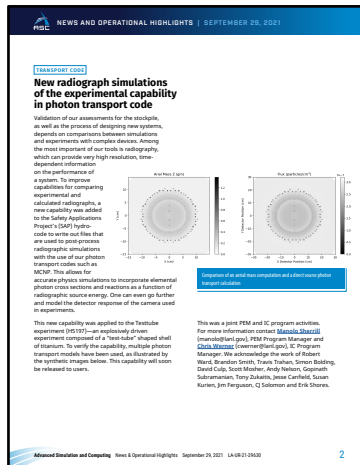
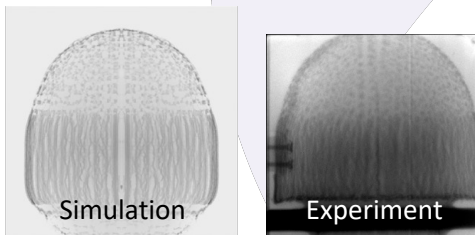
# FY20-21 Highlights

- Mark & Emily joined team
- March 2021: AWS Newsbite
- April 2021: FLIP+MPM Newsbite
- August 2021: Sierra L2 Milestone
- August 2021: LAAP award for infrastructure modernization
- September 2021: Talos Newsbite

Time: 0.0  $\mu$ s



0.0001  
-0.3  
-0.2  
-0.1  
-1.0e+02  
m/s<sup>2</sup> Magnitude



# Collaborations leverage the investment and expertise of others.

- PEM HE: reactive flow models, non-standard HE scenarios, mesoscale HE
- PEM TR: EnSight output, Talos output
- CSSE Production Visualization: ParaView output
- JMP: lagrangian particle hydrodynamics, non-standard HE scenarios, mesoscale HE
- ACQ: lagrangian particle hydrodynamics
- EM: performance improvement
- GS: targeted code needs
- ...
- **Leveraging these funds has allowed meaningful improvement in 3D code performance and successful deployment of focused, unique code capabilities.**

**Collaboration is key to advancing our simulation tools.**



# Code capabilities determine the questions that can be addressed using SAP tools.

## Past: FY20-21

- AWSO reactive burn
- PiSURF • 2D PDV
- 2D synthetic radiograph
- Talos output
- Significant memory reduction of a package
- JWLb for overdriven HE
- Improved initialization, EOS and MATCH temperature support
- Sparse material numbering and improved body naming



## Present: FY22

- rDSD
- PDV robustness
- Full ParaView support
- Viscoelastic brittle failure
- MATCH thermal ignition
- Affine transforms for analysis

## Future

- Implicit hydro and H-S reaction networks
- Memory-efficient STL
- Automatic material priorities
- Gap opening
- Eulerian slidelines
- Improved ceramic and glass models

**Tasks are determined by user needs, staff skills, resources, and programmatic constraints.**

# Infrastructure acts as a force multiplier for software developer skills.

## Past: FY20-21

- ATS-2 nightly testing
- ATS-2 NVHPC nightly build
- Spack environments
- Compiler warnings
- Resolve test diffs
- Finish LaTeX docs
- Git/GitLab migration
- Perl to Python conversion
- Modularize source files

## Present: FY22

- CMake
- GitLab CI on HPC
- Production-level Sierra support

## Future

- Container builds

**Paying down infrastructure debt is complete.**





# Improved code performance allows simulations to finish faster or with greater fidelity.

## Past: FY20-21

- Pre-inverted EOSPAC
- Turn off EOSPAC extrapolation check
- Parallel EnSight output
- Inline Gen
- Automated restart
- Partial GPU support
- Code releases on ATS-2
- Turquoise deployment for DoD
- Remove sync points from EOS evaluation

## Present: FY22

- Profiling and optimization
- Robustness at resolution
- Relax Intel FP model
- Improved interface efficiency to analysis packages
- HDF5 restart

## Future

- Ray-trace Calico
- Vectorization improvements
- Full GPU port
- Flexible mesh management

**Implementation, testing, documentation, and user support are not called out—these are our everyday job.**



# Code performance has dramatically improved over the past ~4 years.

- Performance improvement is an ongoing priority.
- Significant gains have been achieved through vectorization, targeted optimization, improved modeling choices, and removal of synchronization points.
- User-relevant 3D simulations on CTS-1 resources finish in less than a day.
  - 1000  $\mu\text{m}$  & 40 nodes: After 5-9x speedup these simulations finish in **1 hour**.
  - 500  $\mu\text{m}$  & 100 nodes: After another ~3x speedup these simulations finish in **~2 hours**.
  - 250  $\mu\text{m}$  & 100 nodes: In progress...

3D 500  $\mu\text{m}$  benchmark simulation exercised since 2018 is 24% faster in FY21 and a combined 3.4x faster over FY20-FY21. 14% of FY21's improvement is due to avoiding EOSPAC's costly extrapolation check.

